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Comparison of Artificial Neural Network and Multiple Regression Analysis Techniques in Predicting the Mechanical Properties of A356 Alloy

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Abstract

The mechanical properties of aluminium alloy castings, such as EL%, YS and UTS, are controlled by the casting and heat treatment variables, alloy's composition, and melt treatment. Despite the abundance of literature data, the large number of the controlling parameters has made it difficult to predict and model the mechanical properties by the conventional techniques. Another obstacle encountered when making such a prediction is the complex kinetics and interactions that exist among the many variables. The goal of this study was to develop Artificial Neural Network (ANN) and Multiple Regression models to predict the mechanical properties of A356 alloy from the processing variables. Several standard multi-layer ANN models were developed and trained using data from the literature and experimental results. A series of nonlinear regression models were also developed and the results were compared with the predictions made by the ANN models. Due to the complexity of A356's solidification behaviour, the nonlinear regression produced results that were not as accurate as those produced by the ANN model. Unlike the nonlinear regression analysis, ANN can simplify the modelling process by eliminating the need to define a function. The results indicate that ANN is a suitable modelling technique for predicting mechanical properties of castings based on the alloy chemistry and processing variables.

Keywords: Artificial Neural network; Regressionn Analysis; Prediction; Mechanical Properties; Casting, Aluminium Alloys; A356

1. Introduction

Al-Si and Al-Si-Cu alloys have been widely used in various applications because of their high strength-to-weight ratio and good corrosion and casting characteristics. The mechanical properties of cast alloys can be improved by controlling the alloy chemistry as well as casting and heat treatment variables. Heat treatment involves solutionizing at temperatures close to the eutectic temperature followed by quenching and then a combination of natural and artificial aging. The improvement in mechanical properties after heat treatment is mainly due to the formation of precipitates during aging and to the changes in the shape of Si particles. Melt treatments, such as grain refinement (by Ti and B additions), eutectic modification (by Sr or Na additions) or tramp/trace elements (Sn, Sc, Fe, etc.) could also influence the mechanical properties. Other critical variables are the casting microstructure (dendrite arm spacing or DAS, grain size, etc.) and defects (porosity and inclusions), all of which are dictated by the melting and casting processes.

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Due to the large number of controlling metallurgical variables, it is difficult to accurately predict the mechanical properties of aluminium 3xx alloys from these variables. Another obstacle encountered when making such a prediction is the complex kinetics and interactions that exist between the many variables. As a result of these complex interactions, it is difficult to establish the relationships that exist among the variables. It is also important to assess the significance of each variable and their interactions, and leave out those that are not significant. In the present study, two approaches were taken to correlate between the mechanical properties and these controlling variables. Moreover, only the two most common casting methods, i.e., sand and permanent mould casting processes, were considered.

2. Database

The data used in these analyses were collected from published papers on sand and permanent mould cast A356 aluminum alloys [1-13]. Since the mechanical properties are influenced by porosity and inclusions, only the reliable sources, where melts were degassed and melt cleanliness was controlled, were used. The data were collected in such a way to obtain a good range in dependant and independent variables. For the permanent mould, the values of wt%Si and natural aging temperature remained constant at 7 and 25°C, respectively. As a result, the values associated with Si and natural aging temperature did not affect the regression results. Similarly, in the sand mould case four independent variables (Na, Sn, Sb, and natural aging temperature) were fixed. Some of the data used in this work are plotted in Figure 1. It is seen that the data exhibit a wide variation in the yield stress (YS) and ultimate tensile strength (UTS) allowing the analysis to correlate the controlling variables with these properties and establish a predictive model.

3. Mathematical Approaches

3.1 Multiple Linear and Nonlinear Regression Models

As the first step in attempting to predict the mechanical properties of A356 alloy, multiple linear and nonlinear regression analysis techniques were used. Mould type, chemical composition, grain refinement, Si modification, and heat treatment conditions were the model variables. Separate models were developed for YS, UTS and El%. Moreover, sand and permanent mould data were treated separately, and individual models were developed for each case. The weight percent of Si, Cu, Mg, Fe, Ti, Sn and Na or Sr were treated as the independent variables. The heat treatment variables consisted of solutionizing time and temperature, quench temperature, natural aging time, and artificial aging time and temperature. The multiple regression analysis was performed using a Microsoft Excel add-in that generates a model by using the least squares method to fit a line through a set of observations [14]. In the case of nonlinear analysis, a number of functions was defined to describe the relationships between the input and each output variables. Logarithmic terms were used to model certain treatment conditions. The functions for the nonlinear regression model were initially defined according to equation 1:

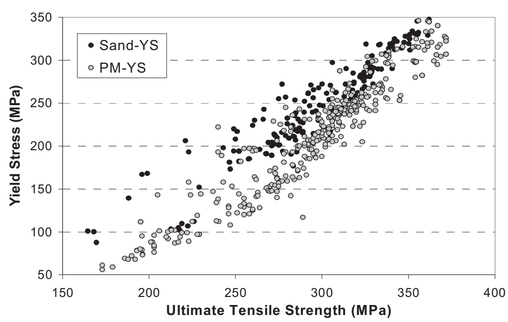

Fig. 1. YS and UTS from literature data for A356 under different casting and heat treatment conditions [1-13].

$$Y = \sum_i \left(a_i x_i + b_i x_i^2\right) + c_i Log(x_i + \varepsilon) + D \tag{1}$$

where Y is the mechanical property, a_i, b_i, c_j, and D are parameters, $\varepsilon = 1.0\text{x}10^{-5}$ to prevent Log(0) from taking place, and x_i represents the input variables (wt%Si, Cu, Mg, Fe, Sr, Na, Ti, Solutionizing time and temperature, natural aging time, artificial aging time and temperature). The logarithmic function was mainly added to better correlate to the precipitation hardening time or temperature. The parameters were calculated by minimizing the adjusted R^2 through an iterative approach. Due to the complexity in developing a nonlinear model with a large number of variables, the number of variables was reduced to create a simpler model without augmenting the error. For example, an analysis of the permanent mould case showed that the weight percent of Cu and Sn did not have much of an impact on the model, and thus were removed from the model. This means that any of the other variables may have a larger influence on the properties and thus the influence of Cu and Sn is minimal, or the data used for the present model did not have a wide enough range. The interactions between variables are also important in developing a nonlinear model. Our analysis showed that the interactions between heat treatment time and temperature are critical, and their interactions can be expressed in the form of $Log(X_i+\varepsilon)*Log(X_j+\varepsilon)$, where the time and temperature are denoted by x_i and x_j, respectively The model with the largest adjusted R^2 value was chosen.

3.2 Artificial Neural Networks (ANN)

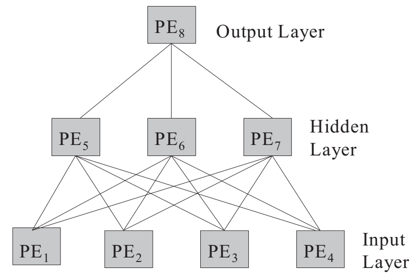

Fig. 2. General structure of an ANN model.

ANN is an important component of modern Artificial Intelligence (AI) computing, which mimics the functions of the human brain and is very effective in learning relationships from complex sets of data [16,17]. Mainly due to its self-learning capability, an ANN can be used for constructing, based solely on observations, a mathematical model for things of a nature, which are not fully understood. Figure 2 is a schematic view of a generalized ANN model, where the input layer is composed of four nodes called processing elements (PEs). A set of data starts its journey at the input layer and then flows into the hidden layer (or layers). The model shown in Figure 2 is made up of one hidden layer with three PEs and an output layer with one PE. Finally, the data flow into the output layer, and the PEs in the hidden and output layers perform the calculations. The weights that connect the different layers are modified in order to minimize the overall error. A commercial artificial intelligence computing package was used to develop the ANN models. The description of the ANN model can be found elsewhere [15].

3.3 Calculation of errors

The standard error of the estimate was used to measure the accuracy of the model predictions. For the regression analyses, the standard error of the estimate, S_e, was calculated according to [18,19]:

$$S_e = \sqrt{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / (n - (k+1))} \tag{2}$$

where y_i is the measured value, $\hat{y}_i$ is the value predicted by the regression analysis, n is the number of data points used, and k is the number of input variables. Note that n-(k+1) is the (residual) degrees of freedom of the model. Unfortunately, the S_e is not suitable for comparing the different models because the degrees of freedom were not available in the case of the ANN models. When comparing the models, it is important to consider the mean value because permanent mould casting gives better mechanical properties (outputs) than that of sand mould, and the three mechanical properties have very different average values. The %El has relatively small values compared to YS and UTS. Since the standard error of the estimate does not take into consideration the mean value of the output, the relative standard error was used to compare the accuracy of the different models. The relative standard error (RSE) was calculated using the following formula [20]:

$$RSE = \frac{S_e}{Mean} \times 100 \tag{3}$$

Whenever the predicted data were compared to the actual data set, a linear least squares fit was calculated and the line was forced to go through the origin. The intercept was set equal to zero because ideally whenever the experimental output is zero, the predicted value should also be zero. The R^2 and adjusted R^2 values were calculated as a tool for analysis of multiple regression model [21-23]. The adjusted R^2 value takes into account the degrees of freedom in the model. Unlike R^2, which increases or remains constant as more input variables are added to the model, the adjusted R^2 can in fact decrease. When there are only a few input variables, R^2 and adjusted R^2 will be very close, but when there are many input variables, the adjusted R^2 might be noticeably lower. Since the adjusted R^2 penalizes complex models, the former is a good tool to compare models with different numbers of input variables [21]. The higher the adjusted R^2 value, the more accurate the model is. It should be noted that a model with many input variables is not necessarily the best model, and thus it is a standard practice to test the significance of each coefficient. In the prsesent study, the input variables were separately removed from the model to see if the adjusted R^2 would improve.

4. Results and Discussion

4.1 Linear and Nonlinear Regression Analysis

Plots of the experimental data against the predictions for YS by linear regression analysis for sand and permanent moulds are shown in Figure 3. In each of the two graphs, the line of best fit is plotted and made to pass through the origin. It seems that predictions are relatively good, but the standard errors are required to compare the predictions.

The values of the standard errors of the estimate of the mechanical properties for multiple linear regression analysis are given in Table 1. The error associated with %El for the permanent mould in Table 1 is higher than that for the sand mould. However, the standard error should be considered in relation to the average EI% values. The average value of %El is higher in the permanent mould than it is in the sand mould. For this reason, the relative standard errors were also calculated (see Table 1). It can be seen that for the permanent mould case, the UTS is predicted relatively well using the multiple linear regression analysis in comparison to the YS and %El values. Based on the relative standard errors, the YS is more precisely predicted than the %El, however, both properties have relative standard errors that are far too high to be considered precise. The same trend is also evident in sand mould case. The table illustrates that for both processes, the UTS has the smallest relative standard error while the %El has the largest relative standard error.

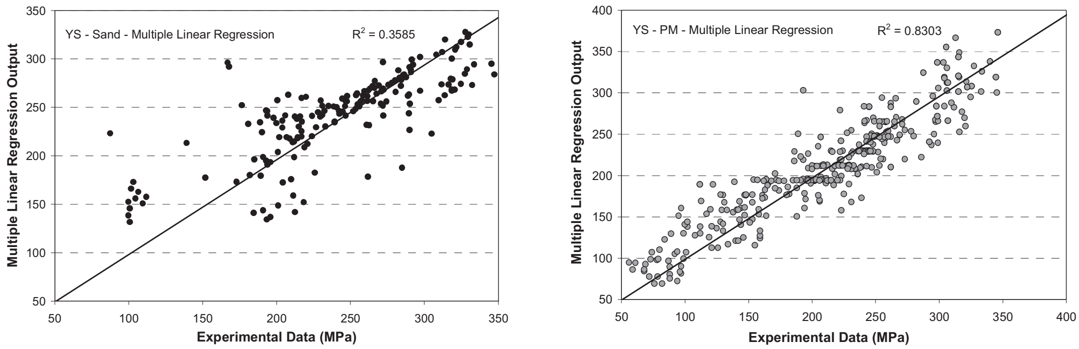

Fig. 3. Comparison of linear regression model predictions vs. actual data of YS for sand and permanent moulds.

Table 1. The standard errors and relative standard error of the estimated mechanical properties from different rent models.

	Standard Error of the Estimate (S_e)						Relative Standard Error (RSE)					
	Sand Mould			Permanent Mould			Sand Mould			Permanent Mould		
Model	*YS*	*UTS*	*%El*	*YS*	*UTS*	*%El*	*YS*	*UTS*	*%El*	*YS*	*UTS*	*%El*
Linear	37.6	29.4	1.5	27.4	20.9	2.7	15.6%	10.0%	34.8%	12.7%	7.1%	19.3%
Nonlinear	21.8	15.1	1.0	20.3	14.7	2.1	9.0%	5.2%	22.4%	9.5%	5.0%	16.1%
ANN	7.7	5.7	0.4	8.1	5.6	0.9	3.2%	1.9%	10%	3.7%	1.8%	6.0%

It can be seen in Table 1 that the relative standard errors of the mechanical properties for the sand mould are significantly higher than those of the permanent mould. This is due to the larger scattering in property data for sand mould compared to permanent mould. Compared to sand castings, the permanent mould castings are sounder, and their properties are higher due to faster solidification rate, with less scattering in property data (lower standard deviation). The relative standard errors in the prediction of %El for sand mould castings are significantly greater than those of the permanent mould castings, but less significant for the YS and UTS. Although some linear relationships may be involved in the prediction of the mechanical properties of A356, linear regression analysis did not provide a good overall prediction of the mechanical properties. Ideally, the model should be able to represent the complex relationships that exist among the variables.

Figure 4 shows how the multiple nonlinear regression analysis performed in comparison to the actual experimental data. The standard errors of the estimate and relative standard errors associated with the nonlinear equations are given in Table 1. Similar to linear regression analysis, the relative standard errors in the prediction of %El for sand mould castings are significantly greater than those of the permanent mould castings, but less significant for the YS and UTS.

A comparison of the relative standard error for linear and nonlinear regression analysis (Table 1) shows that the nonlinear predictions are superior to the linear analysis for all the mechanical properties. Therefore, nonlinear regression analysis provides an overall reasonable prediction of the mechanical properties. The nonlinear regression model was not developed to the fullest extent due to time constrains. The authors tend to explore these avenues even further in their future work. However, small adjustments to the regression models would not dramatically improve their predictive capabilities.

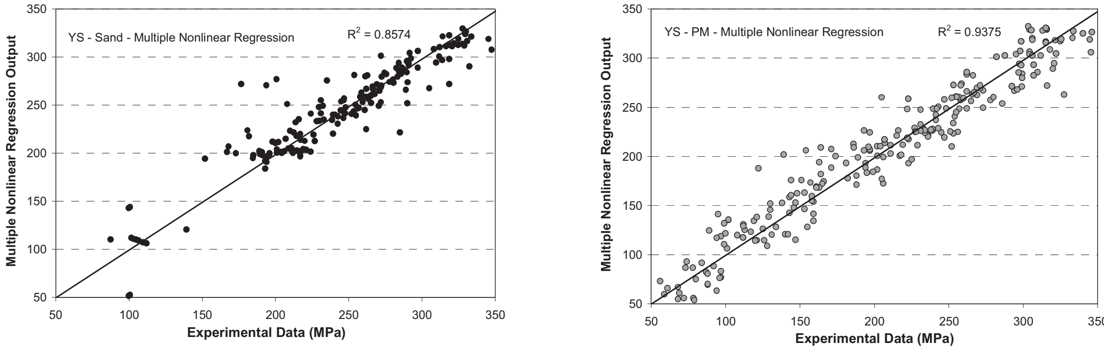

Fig. 4. Comparison of nonlinear regression model predictions vs. actual data of YS for sand and permanent moulds.

4.2 Artificial Neural Network (ANN) Analysis

The data from this study were also used as input into ANN models. The predictive capabilities of the ANN were compared to those of the regression analysis. The ANN models were made up of an input layer, two hidden layers, and an output layer. An iterative approach was applied to optimize the number of PEs and hidden layers. The results indicated that a model with 2 hidden layers would yield optimal results and minimum standard error. The details of the ANN model have been discussed elsewhere [15]. The data set was randomly divided into two segments. One set was used to train the model, whereas the other was used to test it. Figure 5 plots the experimental data against the ANN predictions for YS in both the sand and permanent moulds. It is seen that the ANN predictions are relatively very good. A comparison of the relative standard error in Table 1 shows that the error in ANN prediction of %El for sand mould is slightly higher than that of the permanent mould, but the errors are almost the same for UTS and YS. Although ANN models provided the best results, these models are complicated in their approach and do not permit the user to have a full control of the modelling process, since they act as a black box, and thus render the models hidden.

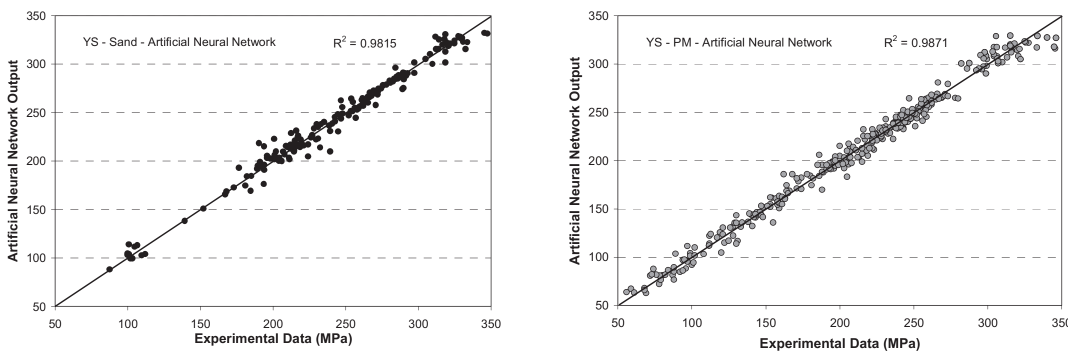

Fig. 5. Comparison of ANN model predictions vs. actual data of YS for sand and permanent moulds.

4.3 Comparison of Regression and ANN Models

A comparison of the models' predictions from Figures 3 to 5, and the relative standard error in Table 1 shows that the ANN method is superior and more accurate than the linear and nonlinear regression analysis for both sand and permanent moulds. The permanent mould process generates more accurate results compared with the sand mould process for all the three models. Moreover, UTS has the smallest relative standard error while %El had the largest relative standard error. The nonlinear regression performed marginally better than the linear regression.

5. Conclusions

Due to the large number of variables and the complex interactions between the variables, conventional modeling techniques are not sufficient to find the correlation between inputs (process variables) and outputs (mechanical properties), and to predict the mechanical properties of the A356 alloy. Multiple linear regression analysis fails to provide accurate predictions of the mechanical properties in sand and permanent moulds because of the interactions between the variables, and the fact that variables do not necessarily follow a linear relationship in their range of interest. The multiple nonlinear regression analysis and Artificial Neural Networks improve the accuracy of the predictions. Among the three models, the ANN had the best predictive capability.

Since Neural Networks have the ability to learn about the complex relationships through successive iterations of the problem at the training stage, as the training stage progresses, the errors are reduced. The training process, the hidden layers, and the weights associated with the neural network allow the model to be developed without a physical understanding or knowing the relationships between the variables. The essence of an accurate model lies in its ability to discern the nature of the relationships that exist among the variables. Linear regression oversimplifies the complex relationships while ANN develops these through the training process.

The nonlinear regression analyses generated models that were less accurate than the ANN model, because the nonlinear regression approach is limited by human capabilities. To perform nonlinear regression analysis, a function must be defined, which requires a physical model. The accuracy of the nonlinear regression analysis depends on whether the specified function describes the underlying physics well. The ANN simplifies the modeling process by eliminating the need for theory, concerning the function. Given the lack of information on relationships and interactions between variables and the three outputs for A356, the ANN generated the most accurate models.

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